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Integral equations for three-body Coulombic resonances*

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Abstract. We propose a novel method for calculating resonances in three-body Coulombic systems. The method is based on the solution of the set of Faddeev and Lippmann-Schwinger integral equations, which are designed for solving the three-body Coulomb problem. The resonances of the three-body system are defined as the complex-energy solutions of the homogeneous Faddeev integral equations. We show how the kernels of the integral equations should be continued analytically in order that we get resonances. As a numerical illustration a toy model for the three-α system is solved.

1 Introduction

For three-body systems the Faddeev equations are the fundamental equations. After one iteration they possess connected kernels, consequently they are effectively Fredholm integral equations of second kind. Thus the Fredholm alternative applies: at certain energy either the homogeneous or inhomogeneous equations have solutions. Three-body bound states correspond to the solutions of the homogeneous Faddeev equations at real energies, resonances, as usual in quantum mechanics, are related to their complex-energy solutions.

The situation becomes more complicated if the Coulomb potential enters into the game. The Faddeev equations were derived for short range interactions and if we simply plug-in a Coulomb-like potential they become singular. The solution has been formulated in the Faddeev-Merkuriev theory [1] on a mathematically sound and elegant way via integral equations with connected (compact) kernels and configuration space differential equations with asymptotic boundary conditions.

*This work is dedicated to the 60th birthday of Prof. W. Glöckle.

Recently, along the concept of a "three-potential" picture, a novel method has been proposed for treating the three-body Coulomb problem via solving the set of Faddeev-Noble and Lippmann-Schwinger integral equations in Coulomb–Sturmian-space representation. The method was elaborated first for bound-state problems [2] with repulsive Coulomb plus nuclear potential, then it was extended for calculating $p-d$ scattering at energies below the breakup threshold [3]. In these calculations an excellent agreements with the results of other well established methods were found and the efficiency and the accuracy of the method were demonstrated. Also atomic bound-state problems with attractive Coulomb interactions were considered [4]. The mathematical validity of the procedure, in the context of the Faddeev-Merkuriev theory, has also been established [5].

In this article we seek to extend this novel method for calculating resonant states, the complex-energy solutions of the homogeneous Faddeev-type integral equations. First, along the method of Ref. [2], we recapitulate the solution of the homogeneous integral equations, then we show how to continue analytically the Green's operators onto the unphysical sheet. As an illustration of the feasibility of this method we calculate a model three-α system interacting via short-range plus repulsive Coulomb interaction.

2 Faddeev-Merkuriev integral equations

The Hamiltonian of a three-body Coulombic system reads

$$H = H^0 + W + v_\alpha + v_\beta + v_\gamma, \tag{1}$$

where H^0 is the three-body kinetic energy operator, W stands for the three-body potential and v_α denotes the Coulomb-like interaction in the subsystem α. We use throughout the usual configuration-space Jacobi coordinates x_α and y_α. Thus v_α only depends on x_α ($v_\alpha = v_\alpha(x_\alpha)$), while W depends on both x_α and y_α coordinates ($W = W(x_\alpha, y_\alpha)$).

The physical role of a Coulomb-like potential is twofold. Its long-distance part modifies the asymptotic motion, while its short-range part strongly correlates the two-body subsystems. Merkuriev proposed to split the potentials into short-range and long-range parts in the three-body configuration space via a cut-off function ζ [1],

$$v_\alpha^{(s)}(x_\alpha, y_\alpha) = v_\alpha(x_\alpha)\zeta_\alpha(x_\alpha, y_\alpha), \tag{2}$$

and

$$v_\alpha^{(l)}(x_\alpha, y_\alpha) = v_\alpha(x_\alpha)[1 - \zeta_\alpha(x_\alpha, y_\alpha)]. \tag{3}$$

The function ζ_α is defined such that it separates the asymptotic two-body sector Ω_α from the rest of the three-body configuration space. On the region of Ω_α the splitting function ζ_α asymptotically tends to 1 and on the complementary asymptotic region of the configuration space it tends to 0. Rigorously, Ω_α is defined as a part of the three-body configuration space where the condition

$$|x_\alpha| < a(1 + |y_\alpha|/a)^\nu, \text{with} \quad a > 0,\ 0 < \nu < 1/2, \tag{4}$$

is satisfied. So, in Ω_α the short-range part $v_\alpha^{(s)}$ coincides with the original Coulomb-like potential v_α and in the complementary region vanishes, whereas the opposite holds true for $v_\alpha^{(l)}$. From its construction follows that if a is chosen big enough $\sum_\alpha v_\alpha^{(l)}$ in the three-body Hilbert space does not support any bound state [1]. This phenomena is analogous to the observation that some special atomic three-body systems does not have any bound states [6]. Note that for repulsive Coulomb interactions one can also adopt Noble's approach [7], which can be considered as a special case of Merkuriev's splitting, where the splitting is performed in the two-body configuration space. Then $v_\alpha^{(l)}$ coincides with the whole Coulomb interaction and $v_\alpha^{(s)}$ with the short range nuclear potential.

In the Faddeev procedure we spilt the wave function into three components

$$|\Psi\rangle = |\psi_\alpha\rangle + |\psi_\beta\rangle + |\psi_\alpha\rangle \tag{5}$$

by applying the asymptotic filtering [8] operator

$$|\psi_\alpha\rangle = G^{(l)}(z) v_\alpha^{(s)} |\Psi\rangle. \tag{6}$$

Here $G^{(l)}$ is the resolvent of the long-ranged Hamiltonian

$$H^{(l)} = H^0 + W + v_\alpha^{(l)} + v_\beta^{(l)} + v_\gamma^{(l)} \tag{7}$$

and z is the complex energy parameter. The wave-function components satisfy the homogeneous Faddeev-Merkuriev integral equations

$$|\psi_\alpha\rangle = G_\alpha^{(l)}(z) v_\alpha^{(s)} \sum_{\gamma \neq \alpha} |\psi_\gamma\rangle, \tag{8}$$

where $G_\alpha^{(l)}$ is the resolvent of the channel long-ranged Hamiltonian

$$H_\alpha^{(l)} = H^{(l)} + v_\alpha^{(s)}. \tag{9}$$

Merkuriev has proved that Egs. (8) possess compact kernels for positive E energies, and this property remains valid also for complex energies $z = E - i\Gamma/2$, $\Gamma > 0$.

3 Solution method

We solve these integral equations in Coulomb–Sturmian-space representation. The Coulomb-Sturmian (CS) functions are defined by

$$\langle r|n\rangle = \left[\frac{n!}{(n+2l+1)!}\right]^{1/2} (2br)^{l+1} \exp(-br) L_n^{2l+1}(2br), \tag{10}$$

with n and l being the radial and orbital angular momentum quantum numbers, respectively, and b is the size parameter of the basis. The CS functions $\{|n\rangle\}$ form a biorthonormal discrete basis in the radial two-body Hilbert space; the

biorthogonal partner defined by $\langle r|\widetilde{n}\rangle = r^{-1}\langle r|n\rangle$. Since the three-body Hilbert space is a direct product of two-body Hilbert spaces, an appropriate basis is the angular momentum coupled direct product (the possible other quantum numbers are implicitly assumed)

$$|n\nu\rangle_\alpha = |n\rangle_\alpha \otimes |\nu\rangle_\alpha, \qquad (n,\nu = 0,1,2,\ldots). \tag{11}$$

With this basis the completeness relation takes the form

$$\mathbf{1} = \lim_{N\to\infty} \sum_{n,\nu=0}^{N} |\widetilde{n\nu}\rangle_\alpha \, {}_\alpha\langle n\nu| = \lim_{N\to\infty} \mathbf{1}_\alpha^N. \tag{12}$$

Note that in the three-body Hilbert space, three equivalent bases belonging to fragmentation α, β and γ are possible.

In Ref. [2] a novel approximation scheme has been proposed to the Faddeev-type integral equations

$$|\psi_\alpha\rangle = G_\alpha^{(l)}(z)\mathbf{1}_\alpha^N v_\alpha^{(s)} \sum_{\gamma\neq\alpha} \mathbf{1}_\gamma^N |\psi_\gamma\rangle, \tag{13}$$

i.e. the short-range potential $v_\alpha^{(s)}$ in the three-body Hilbert space is taken to have a separable form, viz.

$$v_\alpha^{(s)} \approx \sum_{n,\nu,n',\nu'=0}^{N} |\widetilde{n\nu}\rangle_\alpha \, \underline{v}_{\alpha\beta}^{(s)} \, {}_\beta\langle\widetilde{n'\nu'}|, \tag{14}$$

where $\underline{v}_{\alpha\beta}^{(s)} = {}_\alpha\langle n\nu|v_\alpha^{(s)}|n'\nu'\rangle_\beta$. In Ref. [5] the validity of the approximation were proved. The argumentation in Ref. [5] relies on the square integrable property of the term $v_\alpha^{(s)}|\psi_\gamma\rangle$, $\gamma\neq\alpha$. Thus this approximation is justified also for complex energies as long as this property remains valid. In Eq. (14) the ket and bra states are defined for different fragmentation, depending on the environment of the potential operators in the equations. Now, with this approximation, the solution of the homogeneous Faddeev-Merkuriev equations turns into solution of matrix equations for the component vector $\underline{\psi}_\alpha = {}_\alpha\langle\widetilde{n\nu}|\psi_\alpha\rangle$

$$\underline{\psi}_\alpha = \underline{G}_\alpha^{(l)}(z)\underline{v}_\alpha^{(s)} \sum_{\gamma\neq\alpha} \underline{\psi}_\gamma, \tag{15}$$

where $\underline{G}_\alpha^{(l)} = {}_\alpha\langle\widetilde{n\nu}|G_\alpha^{(l)}|\widetilde{n'\nu'}\rangle_\alpha$. A unique solution exists if and only if

$$\det\{[\underline{G}^{(l)}(z)]^{-1} - \underline{v}^{(s)}\} = 0. \tag{16}$$

The Green's operator $G_\alpha^{(l)}$ is a solution of the auxiliary three-body problem with the Hamiltonian $H_\alpha^{(l)}$. To determine it uniquely one should start again from Faddeev-type integral equations, which does not seem to lead any further,

or from the triad of Lippmann-Schwinger equations [9]. The triad of Lippmann-Schwinger equations, although they do not possess compact kernels and thus they are not amenable for practical calculations, also define the solution in an unique way. They are, in fact, related to the adjoint representation of the Faddeev operator [10]. The Hamiltonian $H_\alpha^{(l)}$, however, has a peculiar property that it supports bound state only in the subsystem α, and thus it has only one kind of asymptotic channel, the α channel. For such a system one single Lippmann-Schwinger equation is sufficient for an unique solution [11].

The appropriate equation takes the form

$$G_\alpha^{(l)} = \widetilde{G}_\alpha + \widetilde{G}_\alpha U^\alpha G_\alpha^{(l)}, \tag{17}$$

where $\widetilde{G}_\alpha$ is the resolvent channel-distorted long-range Hamiltonian,

$$\widetilde{H}_\alpha = H^0 + v_\alpha + u_\alpha^{(l)}, \tag{18}$$

and $U^\alpha = W + v_\beta^{(l)} + v_\gamma^{(l)} - u_\alpha^{(l)}$. The auxiliary potential $u_\alpha^{(l)}$ depends on the coordinate y_α. It is defined such that it does not support any bound state and has the asymptotic form $u_\alpha^{(l)} \sim e_\alpha(e_\beta + e_\gamma)/y_\alpha$ as $y_\alpha \to \infty$. In fact, $u_\alpha^{(l)}$ is an effective Coulomb interaction between the center of mass of the subsystem α (with charge $e_\beta + e_\gamma$) and the third particle (with charge e_α). Its role is to compensate the Coulomb tail of the potentials $v_\beta^{(l)} + v_\gamma^{(l)}$ in Ω_α. If $u_\alpha^{(l)}$ is a repulsive Coulomb potential the requirement that it should not support bound states can can easily be fulfilled. For attractive $u_\alpha^{(l)}$ the infinitely many bound states should be projected out, which leads to a non-local potential.

It is important to realize that in this approach to get the solution only the matrix elements $\underline{G}_\alpha^{(l)}$ are needed, i.e. only the representation of the Green's operator on a compact subset of the Hilbert space are required. So, although Eq. (17) does not possesses a compact kernel on the whole three-body Hilbert space its matrix form is effectively a compact equation on the subspace spanned by finite number of CS functions [5]. Thus we can perform an approximation, similar to Eq. (14), on the potential U^α in Eq. (17), with bases of the same fragmentation α applied on both sides of the operator. Now the integral equation reduces to an analogous set of linear algebraic equation with the operators replaced by their matrix representations. The solution is given by

$$[\underline{G}_\alpha^{(l)}(z)]^{-1} = [\underline{\widetilde{G}}_\alpha(z)]^{-1} - \underline{U}^\alpha. \tag{19}$$

The most crucial point in this procedure is the calculation of the matrix elements $\underline{\widetilde{G}}_\alpha = {}_\alpha\langle\widetilde{n\nu}|\widetilde{G}_\alpha|\widetilde{n'\nu'}\rangle_\alpha$, since the potential matrix elements $\underline{v}_{\alpha\beta}^{(s)}$ and $\underline{U}^\alpha$ can always be calculated numerically by making use of the transformation of Jacobi coordinates. The Green's operator $\widetilde{G}_\alpha$ is a resolvent of the sum of two commuting Hamiltonians, $\widetilde{H}_\alpha = h_{x_\alpha} + h_{y_\alpha}$, where $h_{x_\alpha} = h_{x_\alpha}^0 + v_\alpha$ and $h_{y_\alpha} = h_{y_\alpha}^0 + u_\alpha^{(l)}$, which act in different two-body Hilbert spaces. Thus, using the convolution theorem the three-body Green's operator $\widetilde{G}_\alpha$ equates to a

convolution integral of two-body Green's operators, i.e.

$$\widetilde{G}_\alpha(z) = \frac{1}{2\pi \mathrm{i}} \oint_C dz' \, g_{x_\alpha}(z - z') \, g_{y_\alpha}(z'), \tag{20}$$

where $g_{x_\alpha}(z) = (z - h_{x_\alpha})^{-1}$ and $g_{y_\alpha}(z) = (z - h_{y_\alpha})^{-1}$. The contour C should be taken counterclockwise around the continuous spectrum of h_{y_α} so that g_{x_α} is analytic in the domain encircled by C.

To examine the structure of the integrand let us shift the spectrum of g_{x_α} by taking $z = E + \mathrm{i}\varepsilon$ with positive ε. By doing so, the two spectra become well separated and the spectrum of g_{y_α} can be encircled. Next the contour C is deformed analytically in such a way that the upper part descends to the unphysical Riemann sheet of g_{y_α}, while the lower part of C can be detoured away from the cut [see Fig. 1]. The contour still encircles the branch cut singularity of g_{y_α}, but in the $\varepsilon \to 0$ limit it now avoids the singularities of g_{x_α}. Moreover, by continuing to negative values of ε, in order that we can calculate resonances, the branch cut and pole singularities of g_{x_α} move onto the second Riemann sheet of g_{y_α} and, at the same time, the branch cut of g_{y_α} moves onto the second Riemann sheet of g_{x_α}. Thus, the mathematical conditions for the contour integral representation of $\widetilde{G}_\alpha(z)$ in Eq. (20) can be fulfilled also for complex energies with negative imaginary part. In this respect there is only a gradual difference between the bound- and resonant-state calculations. Now, the matrix elements $\underline{\widetilde{G}}_\alpha$ can be cast in the form

$$\underline{\widetilde{G}}_\alpha(z) = \frac{1}{2\pi \mathrm{i}} \oint_C dz' \, \underline{g}_{x_\alpha}(z - z') \, \underline{g}_{y_\alpha}(z'), \tag{21}$$

where the corresponding CS matrix elements of the two-body Green's operators in the integrand are known analytically for all complex energies [12], and thus the convolution integral can be performed also in the practice.

4 Numerical illustration

To illustrate the feasibility of this method we examine the convergence of the results for three-body resonant-state energies. For this purpose we take an Ali–Bodmer-type toy-model for the charged three-α system interacting via s-wave short-range interaction. To improve its properties we add a phenomenological three-body potential. Adopting Noble's splitting we have

$$v_\alpha^{(s)}(r) = V_1 \exp\{-r^2/{\beta_1}^2\} + V_2 \exp\{-r^2/{\beta_2}^2\} \tag{22}$$

with $V_1 = 125$ MeV, $V_2 = -30.18$ MeV, $\beta_1 = 1.53$ fm, $\beta_2 = 2.85$ fm, and

$$v_\alpha^{(l)}(r) = 4e^2/r. \tag{23}$$

We use units such that $\hbar^2/m = 41.47$ MeV, $e^2 = 1.44$ MeV fm. The mass of the α-particle is chosen as $M = 3.973m$, where m denotes the mass of the nucleon. The three body potential is taken to have Gaussian form

$$W(\rho) = V \exp\{-\rho^2/\beta^2\}, \tag{24}$$

where $\rho^2 = \sum_{i=1}^{3} \mathbf{r}_i^2$, $V = -31.935$ MeV and $\beta = 3.315$ fm. Here $\mathbf{r}_i$ stands for the position vector of i-th particle in the center of mass frame of three-α system. We select states with total angular momentum $L = 0$. In Table I we show the convergence of the energy of the ground-state and of the first resonant-state with respect to N, the number of CS functions employed in the expansion. The selected resonance is the experimentally well-known sharp state which has a great relevance in nuclear synthesis.

For comparison we have recalculated the results of Ref. [13], where a two-channel model has been proposed for the three-α system. Table II shows a good agreement between the two independent methods as far as the position of the resonance is considered. For the width of the resonant state we got an order of magnitude less which indicate an order of magnitude longer lifetime. The origin of the discrepancy, in our opinion, could be due to the not proper implementation of the asymptotic boundary conditions in Ref. [13].

5 Conclusions

In this article we have proposed a new method for calculating resonances in three-body Coulombic systems. The homogeneous Faddeev-Merkuriev integral equations were solved for complex energies. For this, being an integral equation approach, the no boundary conditions are needed. The procedure is an extension of the well-established Coulomb-Sturmian separable expansion approach [2, 3, 4]. In fact, the extension is nothing else but the proper analytic continuation of the contour integral representation of the Green's operator. In the non-Coulomb case the method is readily applicable, only the Coulomb Green's operators have to be replaced by the free one.

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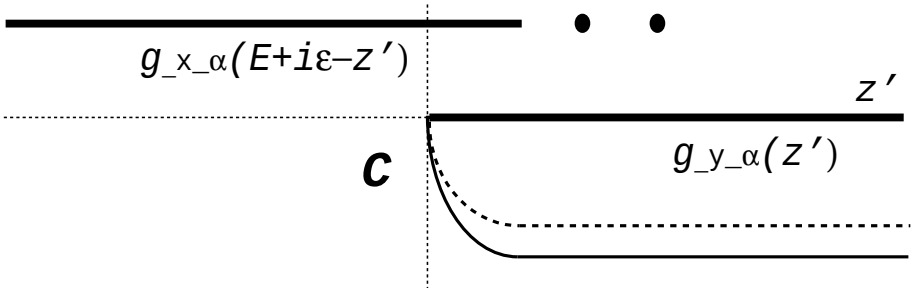

Figure 1. Analytic structure of $g_{x_\alpha}(z-z')\ g_{y_\alpha}(z')$ as a function of z' with $z = E+\mathrm{i}\varepsilon$, $E > 0$, $\varepsilon > 0$. The contour C encircles the continuous spectrum of h_{y_α}. A part of it, which goes on the unphysical Riemann-sheet of g_{y_α}, is drawn by broken line.

Table 1. Convergence of the ground-state and of the first resonant-state energy (in MeV) of a three-α system interacting via the potential of (22) with increasing basis for the separable expansion. N denotes the maximum number of basis states employed for n and ν in Eq. (14).

N	E	$E = E_r - \mathrm{i}\Gamma/2$
15	-7.283686	0.3859108 -i 0.000011
16	-7.283744	0.3854244 -i 0.000011
17	-7.283779	0.3851242 -i 0.000011
18	-7.283801	0.3849323 -i 0.000012
19	-7.283815	0.3848056 -i 0.000012
20	-7.283824	0.3847236 -i 0.000012
21	-7.283829	0.3846683 -i 0.000012
22	-7.283833	0.3846308 -i 0.000012
23	-7.283836	0.3846053 -i 0.000012
24	-7.283837	0.3845873 -i 0.000013
25	-7.283838	0.3845748 -i 0.000013
26	-7.283839	0.3845658 -i 0.000013
27	-7.283840	0.3845593 -i 0.000013
28	-7.283840	0.3845546 -i 0.000013
29	-7.283640	0.3845512 -i 0.000013

Table 2. Results for the three-α model of Ref. [13] (in MeV).

	E	$E = E_r - \mathrm{i}\Gamma/2$	
This work	-6.8053	0.3572	- i 0.000002
Ref. [13]	-6.81	0.38	- i 0.000020

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